



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2022 – 04:34 PM JST

PDB ID : 7YA2
Title : Crystal structure of capsular polysaccharide synthesis enzyme CapG from *Staphylococcus aureus*
Authors : Chen, Y.; Wang, Y.C.
Deposited on : 2022-06-27
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

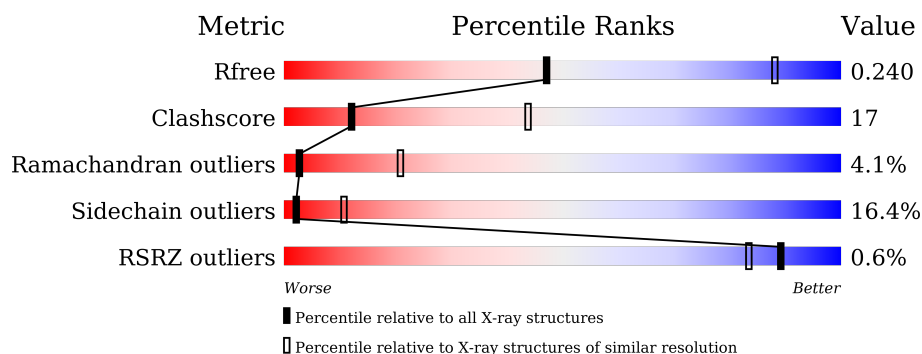
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	374	<div> <div>65%</div> <div>25%</div> <div>9%</div> <div>..</div> </div>
1	B	374	<div> <div>63%</div> <div>28%</div> <div>8%</div> <div>.</div> </div>
1	C	374	<div> <div>57%</div> <div>34%</div> <div>8%</div> <div>.</div> </div>
1	D	374	<div> <div>58%</div> <div>31%</div> <div>10%</div> <div>.</div> </div>
1	E	374	<div> <div>58%</div> <div>32%</div> <div>9%</div> <div>.</div> </div>
1	F	374	<div> <div>54%</div> <div>35%</div> <div>10%</div> <div>.</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18050 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

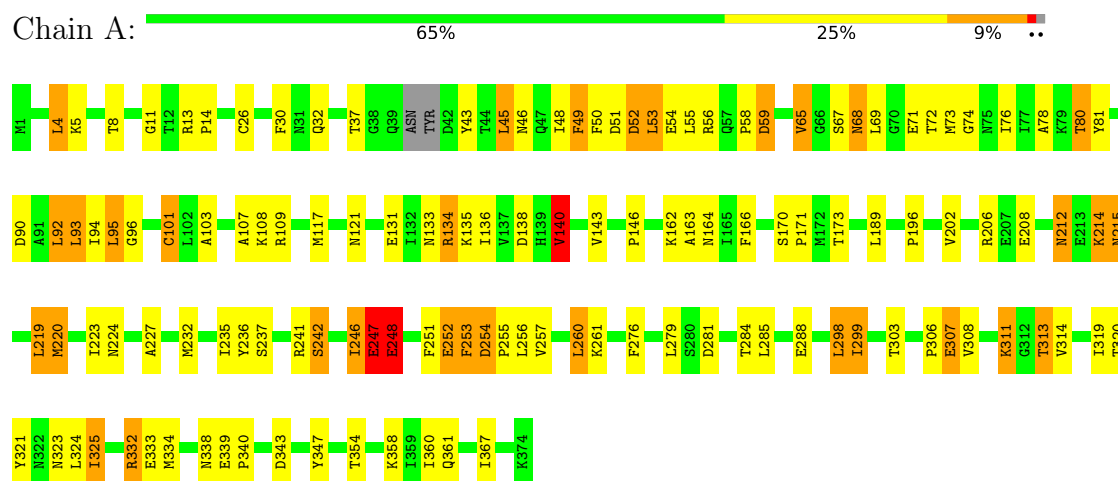
- Molecule 1 is a protein called Capsular polysaccharide synthesis enzyme CapG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2995	1898	512	573	12			
1	B	374	Total	C	N	O	S	0	0	0
			3011	1909	513	577	12			
1	C	374	Total	C	N	O	S	0	0	0
			3011	1909	513	577	12			
1	D	374	Total	C	N	O	S	0	0	0
			3011	1909	513	577	12			
1	E	374	Total	C	N	O	S	0	0	0
			3011	1909	513	577	12			
1	F	374	Total	C	N	O	S	0	0	0
			3011	1909	513	577	12			

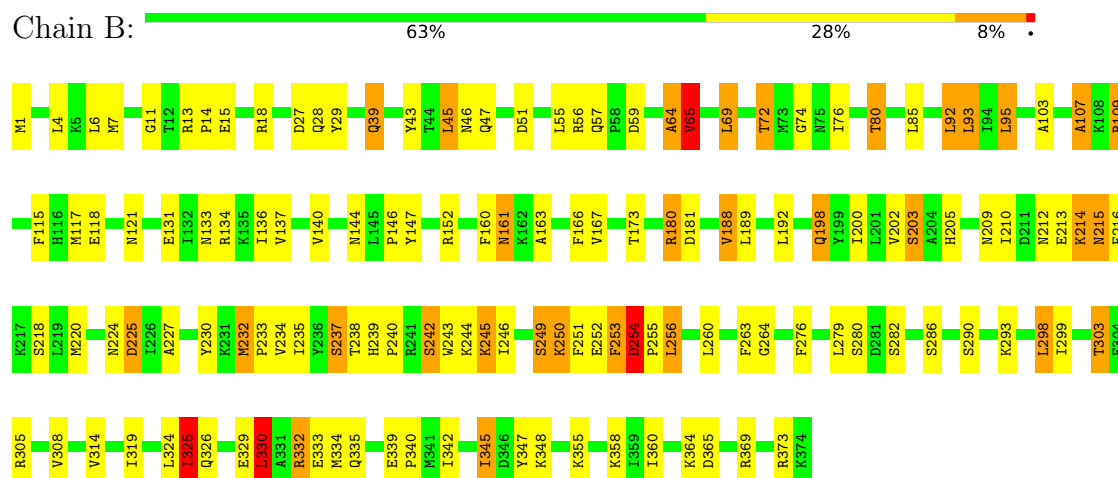
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Capsular polysaccharide synthesis enzyme CapG

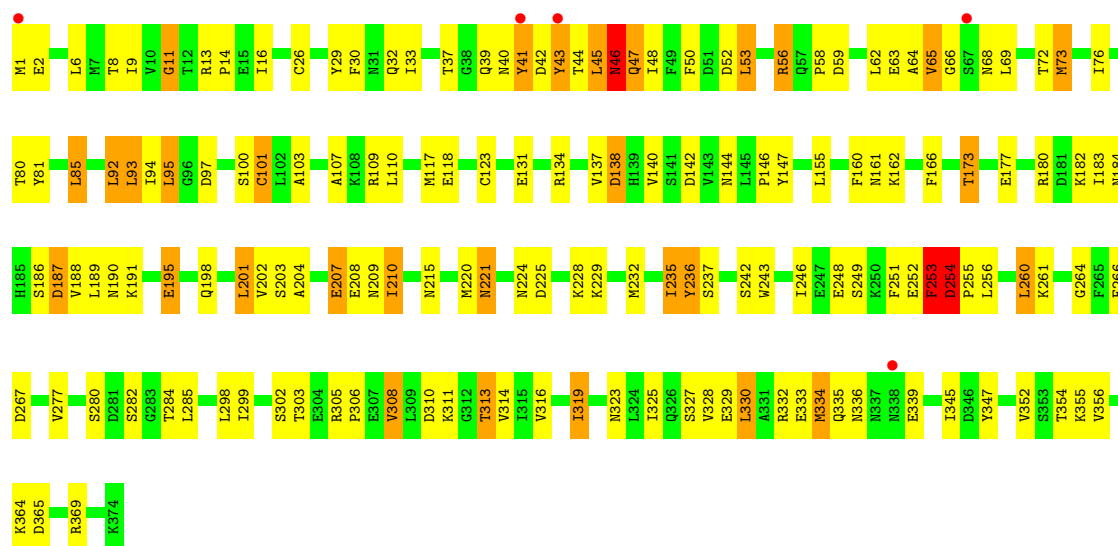


- Molecule 1: Capsular polysaccharide synthesis enzyme CapG

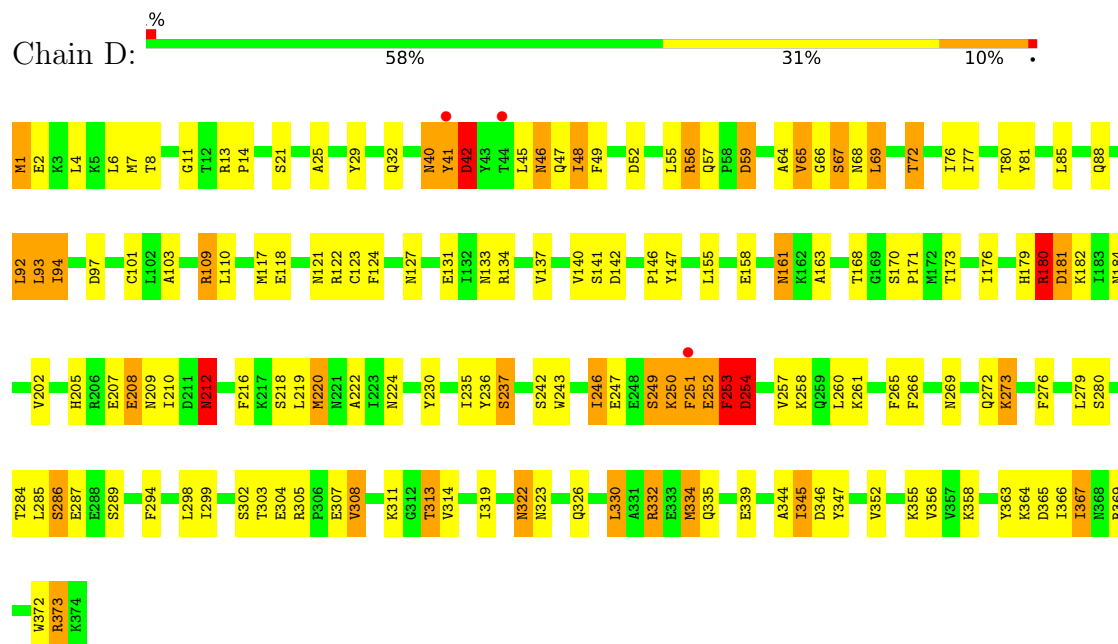


- Molecule 1: Capsular polysaccharide synthesis enzyme CapG

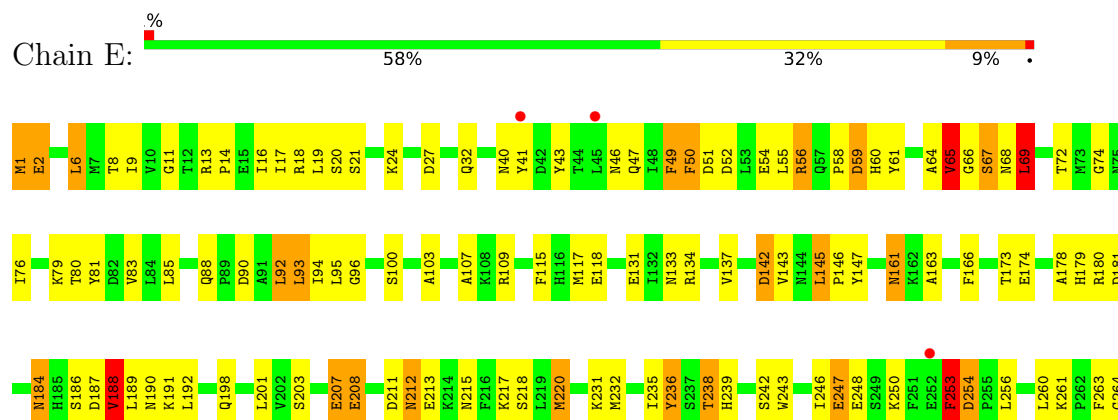


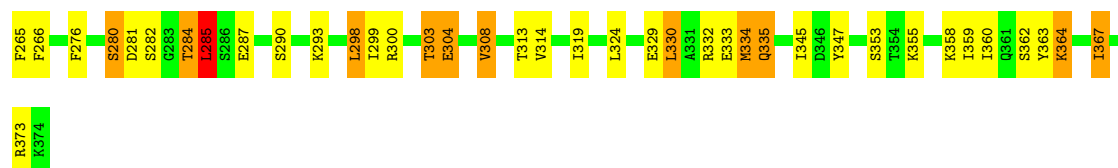


• Molecule 1: Capsular polysaccharide synthesis enzyme CapG

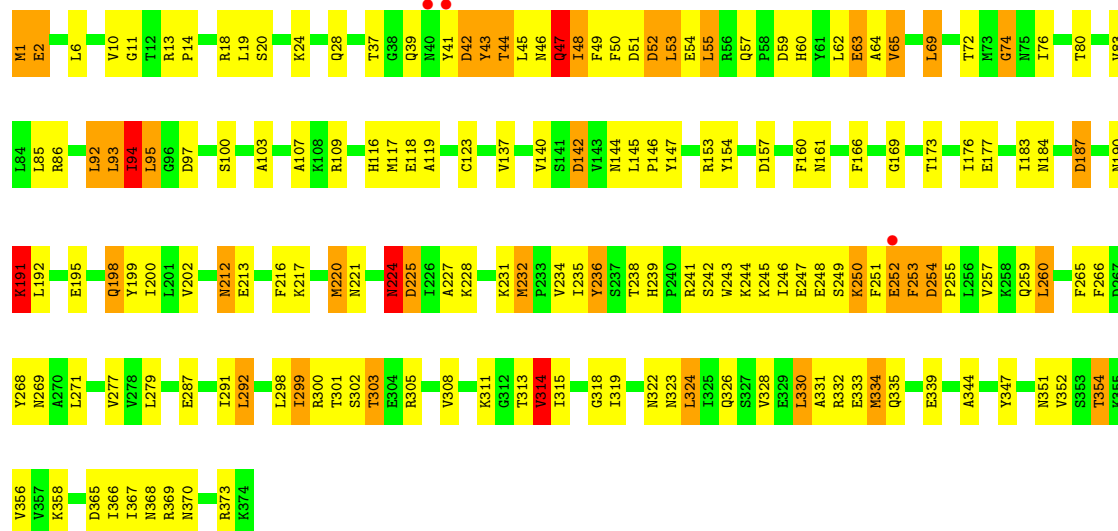


• Molecule 1: Capsular polysaccharide synthesis enzyme CapG





• Molecule 1: Capsular polysaccharide synthesis enzyme CapG



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	302.91Å 84.34Å 145.09Å 90.00° 110.65° 90.00°	Depositor
Resolution (Å)	25.57 – 3.20 25.55 – 3.20	Depositor EDS
% Data completeness (in resolution range)	87.9 (25.57-3.20) 88.1 (25.55-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.17Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.183 , 0.241 0.185 , 0.240	Depositor DCC
R_{free} test set	2558 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18050	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.70	0/3049	0.83	0/4122
1	B	0.71	0/3066	0.82	0/4146
1	C	0.71	0/3066	0.81	0/4146
1	D	0.70	0/3066	0.80	0/4146
1	E	0.70	0/3066	0.79	0/4146
1	F	0.69	0/3066	0.81	0/4146
All	All	0.70	0/18379	0.81	0/24852

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	E	0	3
1	F	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	ASN	Peptide
1	A	96	GLY	Peptide
1	E	253	PHE	Peptide
1	E	41	TYR	Peptide
1	E	50	PHE	Peptide
1	F	52	ASP	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2995	0	3006	105	0
1	B	3011	0	3013	99	0
1	C	3011	0	3013	100	0
1	D	3011	0	3013	114	0
1	E	3011	0	3013	110	0
1	F	3011	0	3013	124	0
All	All	18050	0	18071	616	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (616) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:THR:HG21	1:C:347:TYR:O	1.46	1.13
1:B:95:LEU:HD22	1:B:117:MET:HB3	1.45	0.99
1:A:219:LEU:CD2	1:A:299:ILE:HD11	1.95	0.96
1:A:219:LEU:HD21	1:A:299:ILE:HD11	1.48	0.96
1:C:64:ALA:O	1:C:65:VAL:HG12	1.65	0.95
1:E:76:ILE:O	1:E:80:THR:OG1	1.84	0.93
1:A:235:ILE:HG23	1:A:260:LEU:HG	1.50	0.93
1:A:215:ASN:HD22	1:A:319:ILE:HD13	1.36	0.91
1:B:133:ASN:O	1:B:137:VAL:HG12	1.72	0.90
1:D:173:THR:HG21	1:D:347:TYR:O	1.72	0.90
1:F:173:THR:HG21	1:F:347:TYR:O	1.71	0.89
1:A:242:SER:O	1:A:246:ILE:CG2	2.21	0.89
1:A:219:LEU:HD21	1:A:299:ILE:CD1	2.03	0.88
1:B:46:ASN:HD21	1:B:57:GLN:HE22	1.20	0.87
1:C:235:ILE:HG22	1:C:260:LEU:HG	1.57	0.86
1:A:242:SER:O	1:A:246:ILE:HG23	1.74	0.85
1:A:339:GLU:OE2	1:C:29:TYR:OH	1.96	0.84
1:E:173:THR:HG21	1:E:347:TYR:O	1.78	0.83
1:B:146:PRO:HD2	1:B:166:PHE:O	1.80	0.81
1:C:201:LEU:HD12	1:C:202:VAL:N	1.96	0.80
1:C:243:TRP:O	1:C:246:ILE:HG22	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:ARG:NH1	1:D:59:ASP:OD1	2.16	0.79
1:A:76:ILE:O	1:A:80:THR:HB	1.83	0.79
1:B:95:LEU:CD2	1:B:117:MET:HB3	2.13	0.78
1:B:173:THR:HG21	1:B:347:TYR:O	1.82	0.78
1:C:80:THR:HG21	1:C:103:ALA:HA	1.62	0.78
1:A:215:ASN:HD22	1:A:319:ILE:CD1	1.96	0.78
1:A:80:THR:HG21	1:A:103:ALA:HA	1.65	0.77
1:F:277:VAL:HG11	1:F:328:VAL:HG13	1.68	0.76
1:F:95:LEU:HD22	1:F:117:MET:HB3	1.68	0.76
1:A:143:VAL:HG23	1:A:367:ILE:HD11	1.68	0.75
1:D:76:ILE:O	1:D:80:THR:OG1	2.01	0.75
1:F:92:LEU:HD22	1:F:93:LEU:O	1.85	0.75
1:B:235:ILE:HG22	1:B:260:LEU:HG	1.68	0.75
1:C:195:GLU:HB2	1:C:198:GLN:HG3	1.67	0.75
1:E:304:GLU:N	1:E:304:GLU:OE1	2.20	0.75
1:E:8:THR:OG1	1:E:32:GLN:NE2	2.20	0.74
1:F:254:ASP:OD1	1:F:255:PRO:HD2	1.87	0.74
1:A:253:PHE:O	1:A:254:ASP:O	2.05	0.74
1:D:179:HIS:O	1:D:182:LYS:N	2.19	0.74
1:F:368:ASN:O	1:F:373:ARG:N	2.21	0.74
1:C:187:ASP:O	1:C:189:LEU:N	2.19	0.74
1:B:76:ILE:O	1:B:80:THR:OG1	2.06	0.74
1:E:6:LEU:HD21	1:E:93:LEU:HB2	1.69	0.73
1:F:334:MET:HG3	1:F:339:GLU:HG3	1.68	0.73
1:F:80:THR:HG21	1:F:103:ALA:HA	1.71	0.73
1:E:58:PRO:HG2	1:E:61:TYR:CE2	2.23	0.73
1:E:186:SER:OG	1:E:188:VAL:HG12	1.89	0.73
1:A:50:PHE:O	1:A:54:GLU:HA	1.87	0.73
1:B:43:TYR:O	1:B:47:GLN:HB2	1.88	0.72
1:C:228:LYS:HG2	1:C:254:ASP:OD2	1.90	0.71
1:F:332:ARG:HG3	1:F:333:GLU:N	2.04	0.71
1:F:45:LEU:O	1:F:48:ILE:HG12	1.90	0.71
1:D:358:LYS:HE3	1:F:334:MET:HE3	1.72	0.71
1:D:344:ALA:HB3	1:D:347:TYR:CD2	2.25	0.71
1:D:242:SER:O	1:D:246:ILE:HG23	1.91	0.70
1:D:133:ASN:O	1:D:137:VAL:HG12	1.92	0.70
1:C:56:ARG:NH1	1:C:59:ASP:OD1	2.25	0.70
1:A:358:LYS:HE3	1:E:334:MET:HE3	1.75	0.69
1:D:137:VAL:O	1:D:141:SER:OG	2.08	0.69
1:E:69:LEU:HA	1:E:72:THR:CG2	2.23	0.69
1:A:4:LEU:HD12	1:A:5:LYS:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ASN:HD21	1:F:253:PHE:HA	1.58	0.69
1:C:146:PRO:HD2	1:C:166:PHE:O	1.93	0.69
1:E:284:THR:O	1:E:287:GLU:N	2.25	0.69
1:F:212:ASN:C	1:F:212:ASN:HD22	1.97	0.68
1:F:18:ARG:NH1	1:F:118:GLU:OE1	2.26	0.68
1:A:173:THR:HG21	1:A:347:TYR:O	1.93	0.68
1:A:299:ILE:HG12	1:A:299:ILE:O	1.93	0.68
1:C:235:ILE:CG2	1:C:260:LEU:HG	2.24	0.68
1:D:179:HIS:O	1:D:181:ASP:N	2.27	0.67
1:D:242:SER:C	1:D:246:ILE:HG23	2.15	0.67
1:D:8:THR:OG1	1:D:32:GLN:NE2	2.27	0.67
1:E:13:ARG:HD3	1:E:50:PHE:CE2	2.30	0.67
1:B:243:TRP:HA	1:B:246:ILE:HG12	1.75	0.66
1:B:65:VAL:HA	1:B:72:THR:HB	1.77	0.66
1:A:311:LYS:HA	1:C:355:LYS:HE2	1.77	0.66
1:D:355:LYS:HE2	1:F:311:LYS:HA	1.77	0.66
1:E:220:MET:HE3	1:E:236:TYR:HE2	1.60	0.66
1:A:254:ASP:CG	1:A:255:PRO:HD2	2.16	0.66
1:E:187:ASP:O	1:E:190:ASN:N	2.29	0.66
1:A:339:GLU:HG3	1:A:340:PRO:HD2	1.79	0.65
1:B:95:LEU:HD22	1:B:117:MET:CB	2.24	0.65
1:F:330:LEU:HD22	1:F:334:MET:HE2	1.77	0.65
1:C:80:THR:HG21	1:C:103:ALA:CA	2.27	0.64
1:B:242:SER:C	1:B:246:ILE:HG23	2.18	0.64
1:D:322:ASN:C	1:D:322:ASN:HD22	2.01	0.64
1:F:313:THR:O	1:F:313:THR:HG22	1.97	0.64
1:A:95:LEU:CD2	1:A:117:MET:HB3	2.28	0.64
1:A:219:LEU:CD2	1:A:299:ILE:CD1	2.68	0.64
1:E:118:GLU:HG3	1:E:147:TYR:CE2	2.33	0.63
1:A:361:GLN:HG3	1:E:330:LEU:HD12	1.80	0.63
1:D:142:ASP:HB3	1:D:367:ILE:HD12	1.81	0.63
1:D:6:LEU:HD23	1:D:7:MET:N	2.14	0.62
1:E:178:ALA:O	1:E:179:HIS:ND1	2.31	0.62
1:F:142:ASP:HB3	1:F:367:ILE:HD12	1.81	0.62
1:A:219:LEU:HD23	1:A:299:ILE:HD11	1.82	0.62
1:B:358:LYS:HE2	1:D:334:MET:HE3	1.82	0.62
1:D:224:ASN:ND2	1:D:253:PHE:HB2	2.14	0.62
1:D:289:SER:HB3	1:D:294:PHE:CE1	2.35	0.62
1:E:253:PHE:O	1:E:254:ASP:O	2.18	0.61
1:D:92:LEU:HD23	1:D:93:LEU:N	2.15	0.61
1:B:332:ARG:HG3	1:B:333:GLU:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:CYS:HB2	1:F:302:SER:HB2	1.83	0.61
1:D:64:ALA:O	1:D:65:VAL:HB	2.00	0.61
1:C:94:ILE:HG23	1:C:101:CYS:HB3	1.82	0.60
1:B:242:SER:O	1:B:246:ILE:HG23	2.02	0.60
1:C:311:LYS:HA	1:E:355:LYS:HE2	1.83	0.60
1:E:95:LEU:HD22	1:E:117:MET:HB3	1.82	0.60
1:F:212:ASN:HD22	1:F:213:GLU:N	1.99	0.60
1:D:146:PRO:HG3	1:D:155:LEU:HD12	1.83	0.60
1:D:81:TYR:CZ	1:D:110:LEU:HD21	2.37	0.60
1:E:131:GLU:HA	1:E:134:ARG:HD2	1.82	0.60
1:A:212:ASN:HB3	1:A:215:ASN:OD1	2.01	0.60
1:B:212:ASN:HB3	1:B:215:ASN:HD22	1.66	0.60
1:C:201:LEU:HD12	1:C:202:VAL:H	1.67	0.60
1:E:363:TYR:O	1:E:367:ILE:HG13	2.01	0.59
1:F:69:LEU:HA	1:F:72:THR:CG2	2.32	0.59
1:D:6:LEU:HD21	1:D:93:LEU:HB2	1.84	0.59
1:C:173:THR:CG2	1:C:347:TYR:O	2.38	0.59
1:E:90:ASP:HB3	1:E:364:LYS:HE2	1.83	0.59
1:E:254:ASP:HB3	1:E:256:LEU:HD12	1.85	0.59
1:A:358:LYS:CE	1:E:334:MET:CE	2.81	0.59
1:B:64:ALA:O	1:B:65:VAL:HB	2.01	0.59
1:B:249:SER:OG	1:B:250:LYS:N	2.36	0.59
1:E:64:ALA:O	1:E:65:VAL:HB	2.03	0.59
1:C:40:ASN:O	1:C:43:TYR:N	2.30	0.58
1:C:308:VAL:HG13	1:C:313:THR:HG22	1.85	0.58
1:A:92:LEU:HD12	1:A:107:ALA:HB2	1.84	0.58
1:A:146:PRO:HD2	1:A:166:PHE:O	2.02	0.58
1:B:39:GLN:HE21	1:B:39:GLN:C	2.06	0.58
1:D:330:LEU:HD22	1:D:334:MET:HE2	1.86	0.58
1:E:85:LEU:O	1:E:88:GLN:HG2	2.02	0.58
1:A:68:ASN:ND2	1:A:71:GLU:H	2.02	0.58
1:A:232:MET:C	1:A:256:LEU:HD23	2.23	0.57
1:B:152:ARG:NH2	1:B:167:VAL:HG23	2.19	0.57
1:F:199:TYR:OH	1:F:271:LEU:O	2.22	0.57
1:C:94:ILE:CG2	1:C:101:CYS:HB3	2.35	0.57
1:E:68:ASN:O	1:E:72:THR:HG22	2.05	0.57
1:A:358:LYS:HE3	1:E:334:MET:CE	2.35	0.57
1:D:45:LEU:HA	1:D:48:ILE:CG2	2.35	0.57
1:E:51:ASP:O	1:E:54:GLU:N	2.37	0.57
1:E:1:MET:HG2	1:E:2:GLU:H	1.70	0.56
1:D:276:PHE:CZ	1:D:332:ARG:HB2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASP:OD2	1:A:255:PRO:HD2	2.05	0.56
1:B:118:GLU:HG3	1:B:147:TYR:CE2	2.41	0.56
1:D:173:THR:CG2	1:D:347:TYR:O	2.52	0.56
1:F:352:VAL:O	1:F:356:VAL:HG23	2.05	0.56
1:A:284:THR:O	1:A:288:GLU:CG	2.53	0.56
1:B:235:ILE:CG2	1:B:260:LEU:HG	2.36	0.56
1:F:217:LYS:O	1:F:221:ASN:HB2	2.06	0.56
1:A:202:VAL:HG11	1:A:223:ILE:HD11	1.88	0.56
1:E:329:GLU:O	1:E:333:GLU:HB2	2.05	0.56
1:C:334:MET:HG3	1:C:339:GLU:HG3	1.88	0.56
1:F:323:ASN:O	1:F:326:GLN:N	2.38	0.56
1:B:276:PHE:CZ	1:B:332:ARG:HB2	2.40	0.55
1:A:131:GLU:HA	1:A:134:ARG:HD2	1.88	0.55
1:D:216:PHE:HZ	1:D:246:ILE:HG22	1.71	0.55
1:C:80:THR:HG21	1:C:103:ALA:CB	2.36	0.55
1:D:334:MET:HG3	1:D:339:GLU:HG3	1.87	0.55
1:D:220:MET:HE3	1:D:236:TYR:CE2	2.42	0.55
1:A:95:LEU:HD22	1:A:117:MET:HB3	1.88	0.55
1:A:235:ILE:CG2	1:A:260:LEU:HG	2.30	0.54
1:A:56:ARG:NH1	1:A:59:ASP:OD2	2.39	0.54
1:D:237:SER:HB2	1:D:260:LEU:HD12	1.89	0.54
1:E:220:MET:HE3	1:E:236:TYR:CE2	2.40	0.54
1:C:52:ASP:O	1:C:53:LEU:HB2	2.06	0.54
1:F:92:LEU:HD12	1:F:107:ALA:CB	2.38	0.54
1:D:253:PHE:O	1:D:254:ASP:O	2.24	0.54
1:E:80:THR:HG21	1:E:103:ALA:CB	2.38	0.54
1:C:11:GLY:HA3	1:C:100:SER:OG	2.07	0.54
1:A:68:ASN:ND2	1:A:68:ASN:O	2.37	0.54
1:A:321:TYR:CZ	1:A:325:ILE:HD11	2.43	0.54
1:F:137:VAL:HA	1:F:140:VAL:CG1	2.37	0.54
1:C:203:SER:O	1:C:280:SER:HA	2.07	0.53
1:E:49:PHE:HB3	1:E:50:PHE:HD2	1.71	0.53
1:F:10:VAL:HG12	1:F:19:LEU:HD12	1.90	0.53
1:B:237:SER:CB	1:B:260:LEU:HD12	2.38	0.53
1:C:215:ASN:CG	1:C:319:ILE:HG21	2.28	0.53
1:D:118:GLU:HG3	1:D:147:TYR:CE2	2.43	0.53
1:E:18:ARG:NH1	1:E:118:GLU:OE1	2.41	0.53
1:E:81:TYR:CZ	1:F:69:LEU:O	2.61	0.53
1:F:235:ILE:CG2	1:F:260:LEU:HG	2.38	0.53
1:A:67:SER:O	1:A:68:ASN:ND2	2.42	0.53
1:A:206:ARG:HD3	1:A:281:ASP:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:GLU:O	1:C:198:GLN:HB2	2.09	0.53
1:E:282:SER:OG	1:E:284:THR:OG1	2.26	0.53
1:F:253:PHE:O	1:F:254:ASP:CB	2.57	0.53
1:B:27:ASP:OD1	1:B:56:ARG:NH2	2.42	0.53
1:A:299:ILE:O	1:A:299:ILE:CG1	2.57	0.53
1:B:239:HIS:HB3	1:B:240:PRO:HD2	1.90	0.53
1:D:365:ASP:OD2	1:F:323:ASN:ND2	2.42	0.53
1:E:95:LEU:CD2	1:E:117:MET:HB3	2.39	0.53
1:F:146:PRO:HD2	1:F:166:PHE:O	2.08	0.53
1:C:50:PHE:CE1	1:C:58:PRO:HD3	2.44	0.53
1:D:249:SER:OG	1:D:250:LYS:N	2.39	0.53
1:E:59:ASP:O	1:E:60:HIS:CD2	2.62	0.53
1:E:298:LEU:HD22	1:E:300:ARG:HB2	1.90	0.53
1:D:13:ARG:HD3	1:D:49:PHE:CE2	2.44	0.53
1:F:137:VAL:HA	1:F:140:VAL:HG12	1.91	0.53
1:D:137:VAL:HA	1:D:140:VAL:HG12	1.91	0.53
1:E:133:ASN:O	1:E:137:VAL:HG12	2.09	0.53
1:F:247:GLU:OE2	1:F:247:GLU:HA	2.08	0.53
1:F:315:ILE:HD13	1:F:330:LEU:HD13	1.91	0.53
1:B:246:ILE:HB	1:B:253:PHE:HZ	1.74	0.52
1:D:142:ASP:HB3	1:D:367:ILE:CD1	2.39	0.52
1:A:94:ILE:HG23	1:A:101:CYS:HB3	1.90	0.52
1:B:202:VAL:HG22	1:B:279:LEU:HB2	1.91	0.52
1:C:204:ALA:O	1:C:210:ILE:HD11	2.09	0.52
1:C:255:PRO:HD2	1:C:256:LEU:HD12	1.92	0.52
1:E:115:PHE:CE2	1:E:143:VAL:HG21	2.44	0.52
1:A:298:LEU:HD22	1:A:298:LEU:C	2.30	0.52
1:B:254:ASP:CB	1:B:255:PRO:HD2	2.40	0.52
1:D:4:LEU:N	1:F:326:GLN:NE2	2.57	0.52
1:C:95:LEU:HD22	1:C:117:MET:HB3	1.92	0.52
1:D:182:LYS:HD2	1:D:266:PHE:CE2	2.44	0.52
1:E:56:ARG:HD3	1:E:56:ARG:C	2.29	0.52
1:F:52:ASP:O	1:F:53:LEU:HB2	2.10	0.52
1:D:68:ASN:O	1:D:72:THR:HG22	2.10	0.52
1:D:305:ARG:NE	1:D:307:GLU:OE2	2.37	0.52
1:A:95:LEU:HD22	1:A:117:MET:CB	2.39	0.52
1:F:299:ILE:HG23	1:F:324:LEU:HD21	1.91	0.52
1:F:315:ILE:CD1	1:F:330:LEU:HD13	2.40	0.52
1:B:46:ASN:ND2	1:B:57:GLN:HE22	1.98	0.52
1:C:45:LEU:C	1:C:47:GLN:H	2.12	0.52
1:D:305:ARG:HD3	1:D:347:TYR:OH	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ASN:O	1:D:122:ARG:HD3	2.09	0.51
1:B:64:ALA:O	1:B:65:VAL:CB	2.58	0.51
1:A:4:LEU:HD12	1:A:4:LEU:C	2.31	0.51
1:C:138:ASP:OD2	1:C:155:LEU:HD21	2.10	0.51
1:D:253:PHE:CZ	1:D:257:VAL:HG11	2.45	0.51
1:D:308:VAL:HG22	1:D:313:THR:CG2	2.41	0.51
1:E:142:ASP:HB3	1:E:367:ILE:HD13	1.92	0.51
1:D:207:GLU:O	1:D:208:GLU:CB	2.58	0.51
1:B:224:ASN:O	1:B:227:ALA:HB3	2.10	0.51
1:C:221:ASN:O	1:C:224:ASN:HB3	2.09	0.51
1:B:334:MET:HE3	1:F:358:LYS:CE	2.40	0.51
1:F:313:THR:O	1:F:314:VAL:HB	2.10	0.51
1:D:224:ASN:HD21	1:D:253:PHE:CB	2.23	0.51
1:F:13:ARG:HB2	1:F:14:PRO:HD3	1.91	0.51
1:F:80:THR:HG21	1:F:103:ALA:CA	2.41	0.51
1:E:145:LEU:HD21	1:E:359:ILE:HG21	1.93	0.51
1:F:300:ARG:O	1:F:318:GLY:HA2	2.11	0.51
1:B:212:ASN:HB3	1:B:215:ASN:ND2	2.25	0.51
1:E:236:TYR:CE1	1:E:238:THR:HB	2.46	0.51
1:F:268:TYR:O	1:F:271:LEU:HB3	2.10	0.51
1:A:339:GLU:CG	1:C:354:THR:HG21	2.41	0.50
1:A:358:LYS:HE2	1:E:334:MET:CE	2.41	0.50
1:F:311:LYS:HG3	1:F:344:ALA:HA	1.94	0.50
1:A:68:ASN:HD21	1:A:71:GLU:H	1.59	0.50
1:B:232:MET:O	1:B:256:LEU:HD12	2.11	0.50
1:D:330:LEU:O	1:D:334:MET:HB2	2.11	0.50
1:E:198:GLN:HA	1:E:198:GLN:HE21	1.76	0.50
1:E:49:PHE:HB3	1:E:50:PHE:CD2	2.46	0.50
1:A:298:LEU:HD22	1:A:299:ILE:N	2.27	0.50
1:C:277:VAL:HG11	1:C:328:VAL:HG13	1.92	0.50
1:E:64:ALA:HA	1:E:79:LYS:HE3	1.92	0.50
1:A:74:GLY:HA2	1:B:74:GLY:HA2	1.94	0.50
1:A:358:LYS:CE	1:E:334:MET:HE3	2.38	0.50
1:B:237:SER:HB2	1:B:260:LEU:HD12	1.92	0.50
1:E:142:ASP:HB3	1:E:367:ILE:CD1	2.42	0.50
1:E:276:PHE:CZ	1:E:332:ARG:HB2	2.47	0.50
1:F:227:ALA:HB2	1:F:234:VAL:HG21	1.93	0.50
1:F:53:LEU:HD23	1:F:55:LEU:HD12	1.93	0.50
1:C:64:ALA:O	1:C:65:VAL:CG1	2.51	0.50
1:C:137:VAL:HA	1:C:140:VAL:HG12	1.92	0.50
1:E:17:ILE:O	1:E:20:SER:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:CYS:HB2	1:D:302:SER:HB2	1.93	0.50
1:D:272:GLN:HB3	1:D:294:PHE:CE2	2.47	0.50
1:F:243:TRP:CZ2	1:F:259:GLN:HG2	2.47	0.50
1:E:355:LYS:O	1:E:359:ILE:HG13	2.12	0.49
1:E:80:THR:HG21	1:E:103:ALA:HB1	1.92	0.49
1:E:281:ASP:HB3	1:E:299:ILE:HG13	1.92	0.49
1:F:51:ASP:O	1:F:54:GLU:N	2.45	0.49
1:A:232:MET:O	1:A:256:LEU:HD23	2.12	0.49
1:B:332:ARG:CG	1:B:333:GLU:N	2.74	0.49
1:B:345:ILE:HA	1:B:348:LYS:HE3	1.95	0.49
1:D:322:ASN:HD22	1:D:323:ASN:N	2.08	0.49
1:E:161:ASN:HD22	1:E:163:ALA:H	1.60	0.49
1:F:92:LEU:HD12	1:F:107:ALA:HB2	1.93	0.49
1:C:310:ASP:O	1:E:355:LYS:HD3	2.12	0.49
1:D:216:PHE:CZ	1:D:246:ILE:HG22	2.47	0.49
1:F:299:ILE:CG2	1:F:324:LEU:HD21	2.43	0.49
1:D:142:ASP:CB	1:D:367:ILE:HD12	2.43	0.49
1:D:147:TYR:CE1	1:D:171:PRO:HD3	2.47	0.49
1:C:311:LYS:HE2	1:C:345:ILE:HD12	1.94	0.49
1:E:14:PRO:O	1:E:18:ARG:HG3	2.13	0.49
1:E:13:ARG:HB2	1:E:14:PRO:HD3	1.94	0.49
1:C:183:ILE:HG22	1:C:184:ASN:HD22	1.76	0.49
1:A:255:PRO:HG2	1:A:256:LEU:HD12	1.95	0.49
1:C:236:TYR:O	1:C:260:LEU:HB2	2.12	0.49
1:D:80:THR:HG21	1:D:103:ALA:CB	2.42	0.49
1:E:215:ASN:ND2	1:E:319:ILE:HG21	2.28	0.49
1:F:147:TYR:O	1:F:169:GLY:HA2	2.13	0.49
1:F:200:ILE:HG13	1:F:232:MET:HE2	1.94	0.49
1:A:95:LEU:CD2	1:A:117:MET:CB	2.91	0.49
1:A:163:ALA:C	1:A:164:ASN:HD22	2.17	0.49
1:B:210:ILE:HD11	1:B:238:THR:OG1	2.13	0.49
1:B:242:SER:O	1:B:246:ILE:N	2.45	0.49
1:A:253:PHE:C	1:A:254:ASP:O	2.50	0.48
1:E:16:ILE:O	1:E:20:SER:N	2.47	0.48
1:B:161:ASN:C	1:B:161:ASN:HD22	2.15	0.48
1:C:316:VAL:HB	1:E:362:SER:HB3	1.95	0.48
1:E:184:ASN:N	1:E:184:ASN:HD22	2.12	0.48
1:F:254:ASP:OD1	1:F:255:PRO:CD	2.60	0.48
1:F:313:THR:O	1:F:313:THR:CG2	2.61	0.48
1:A:220:MET:HE3	1:A:236:TYR:CE2	2.49	0.48
1:B:115:PHE:CE2	1:B:360:ILE:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:CYS:HB2	1:C:302:SER:HB2	1.94	0.48
1:C:144:ASN:O	1:C:146:PRO:HD3	2.14	0.48
1:C:207:GLU:O	1:C:208:GLU:HB2	2.14	0.48
1:B:203:SER:O	1:B:280:SER:HA	2.14	0.48
1:B:242:SER:O	1:B:245:LYS:N	2.47	0.48
1:B:243:TRP:O	1:B:246:ILE:HG13	2.14	0.48
1:B:334:MET:HE3	1:F:358:LYS:HE3	1.94	0.48
1:B:355:LYS:HE2	1:D:311:LYS:HA	1.95	0.48
1:C:68:ASN:O	1:C:72:THR:HG22	2.13	0.48
1:E:207:GLU:O	1:E:208:GLU:CB	2.61	0.48
1:E:280:SER:HB3	1:E:285:LEU:HG	1.96	0.48
1:D:161:ASN:HD22	1:D:163:ALA:H	1.61	0.48
1:E:246:ILE:C	1:E:246:ILE:HD12	2.34	0.48
1:B:131:GLU:HA	1:B:134:ARG:HD2	1.96	0.48
1:B:254:ASP:HB2	1:B:255:PRO:HD2	1.94	0.48
1:B:298:LEU:CD1	1:B:303:THR:HG23	2.44	0.48
1:C:330:LEU:HD22	1:C:334:MET:CE	2.43	0.48
1:D:207:GLU:O	1:D:208:GLU:HB2	2.14	0.48
1:A:133:ASN:O	1:A:135:LYS:N	2.47	0.48
1:C:65:VAL:HA	1:C:72:THR:OG1	2.14	0.48
1:F:43:TYR:O	1:F:46:ASN:N	2.47	0.48
1:F:235:ILE:HD13	1:F:235:ILE:N	2.29	0.48
1:A:284:THR:O	1:A:288:GLU:HG2	2.13	0.47
1:F:199:TYR:N	1:F:232:MET:HE1	2.29	0.47
1:A:247:GLU:O	1:A:248:GLU:C	2.52	0.47
1:B:214:LYS:O	1:B:216:PHE:N	2.47	0.47
1:B:358:LYS:CE	1:D:334:MET:HE3	2.43	0.47
1:C:253:PHE:O	1:C:253:PHE:CD2	2.67	0.47
1:D:93:LEU:HD21	1:D:117:MET:HE2	1.96	0.47
1:D:212:ASN:C	1:D:212:ASN:HD22	2.18	0.47
1:E:27:ASP:OD1	1:E:56:ARG:NH2	2.47	0.47
1:A:48:ILE:HA	1:A:52:ASP:HB2	1.96	0.47
1:A:68:ASN:C	1:A:68:ASN:HD22	2.17	0.47
1:F:190:ASN:O	1:F:192:LEU:N	2.48	0.47
1:D:224:ASN:ND2	1:D:253:PHE:CB	2.77	0.47
1:F:69:LEU:HA	1:F:72:THR:HG22	1.96	0.47
1:F:93:LEU:O	1:F:94:ILE:HG13	2.14	0.47
1:F:95:LEU:HD22	1:F:117:MET:CB	2.42	0.47
1:F:303:THR:HB	1:F:305:ARG:H	1.80	0.47
1:B:198:GLN:O	1:B:233:PRO:HD2	2.14	0.47
1:C:95:LEU:HD22	1:C:117:MET:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ARG:NH2	1:D:158:GLU:OE1	2.47	0.47
1:D:247:GLU:HA	1:D:251:PHE:CB	2.45	0.47
1:F:80:THR:HA	1:F:83:VAL:HG12	1.97	0.47
1:A:214:LYS:HD2	1:A:214:LYS:O	2.15	0.47
1:C:186:SER:OG	1:C:267:ASP:OD1	2.31	0.47
1:E:174:GLU:OE2	1:E:353:SER:OG	2.22	0.47
1:F:62:LEU:O	1:F:63:GLU:C	2.52	0.47
1:F:332:ARG:HG3	1:F:333:GLU:H	1.77	0.47
1:A:68:ASN:ND2	1:A:68:ASN:C	2.68	0.47
1:B:13:ARG:HB2	1:B:14:PRO:HD3	1.97	0.47
1:C:236:TYR:HD1	1:C:237:SER:N	2.12	0.47
1:E:207:GLU:O	1:E:208:GLU:CG	2.63	0.47
1:A:8:THR:CB	1:A:32:GLN:HE21	2.28	0.47
1:A:308:VAL:HG22	1:A:313:THR:HG21	1.97	0.47
1:C:40:ASN:O	1:C:42:ASP:N	2.47	0.47
1:A:92:LEU:HD23	1:A:93:LEU:N	2.31	0.46
1:A:279:LEU:CD2	1:A:324:LEU:HD22	2.45	0.46
1:E:20:SER:OG	1:E:21:SER:N	2.47	0.46
1:B:14:PRO:O	1:B:18:ARG:HG3	2.14	0.46
1:C:305:ARG:N	1:C:306:PRO:CD	2.78	0.46
1:D:345:ILE:HG22	1:D:346:ASP:N	2.31	0.46
1:F:42:ASP:O	1:F:44:THR:N	2.48	0.46
1:A:4:LEU:HD21	1:A:360:ILE:HG22	1.97	0.46
1:C:69:LEU:O	1:D:81:TYR:CZ	2.69	0.46
1:C:46:ASN:H	1:C:46:ASN:HD22	1.64	0.46
1:F:64:ALA:O	1:F:65:VAL:HB	2.16	0.46
1:B:14:PRO:O	1:B:18:ARG:CG	2.64	0.46
1:E:146:PRO:HD2	1:E:166:PHE:O	2.16	0.46
1:F:10:VAL:HG12	1:F:19:LEU:CD1	2.46	0.46
1:A:276:PHE:CE2	1:A:332:ARG:HG2	2.51	0.46
1:B:239:HIS:O	1:B:243:TRP:CD1	2.68	0.46
1:C:187:ASP:O	1:C:190:ASN:N	2.48	0.46
1:D:47:GLN:OE1	1:D:57:GLN:NE2	2.48	0.46
1:C:352:VAL:O	1:C:356:VAL:HG23	2.15	0.46
1:E:308:VAL:HG22	1:E:313:THR:CG2	2.46	0.46
1:A:108:LYS:HD3	1:A:140:VAL:O	2.16	0.45
1:C:9:ILE:HD12	1:C:92:LEU:HD21	1.97	0.45
1:E:187:ASP:O	1:E:189:LEU:N	2.49	0.45
1:E:308:VAL:HG22	1:E:313:THR:HG21	1.98	0.45
1:F:59:ASP:C	1:F:60:HIS:CD2	2.90	0.45
1:A:46:ASN:O	1:A:49:PHE:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:GLU:HA	1:D:134:ARG:HD2	1.98	0.45
1:D:235:ILE:HG23	1:D:260:LEU:HG	1.96	0.45
1:E:6:LEU:HD21	1:E:93:LEU:CB	2.44	0.45
1:A:361:GLN:HG3	1:E:330:LEU:CD1	2.46	0.45
1:B:4:LEU:N	1:D:326:GLN:NE2	2.64	0.45
1:E:247:GLU:C	1:E:248:GLU:HG3	2.36	0.45
1:D:243:TRP:O	1:D:246:ILE:HG13	2.17	0.45
1:F:299:ILE:O	1:F:300:ARG:HG3	2.16	0.45
1:B:80:THR:HG21	1:B:103:ALA:CB	2.46	0.45
1:D:273:LYS:HA	1:D:294:PHE:HD2	1.82	0.45
1:D:372:TRP:O	1:D:373:ARG:O	2.33	0.45
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.83	0.45
1:C:334:MET:HE3	1:E:358:LYS:HE3	1.98	0.45
1:F:46:ASN:O	1:F:47:GLN:C	2.54	0.45
1:B:28:GLN:HB2	1:B:29:TYR:CD2	2.52	0.45
1:F:248:GLU:O	1:F:251:PHE:HD2	2.00	0.45
1:B:329:GLU:O	1:B:330:LEU:C	2.55	0.45
1:E:9:ILE:HG13	1:E:92:LEU:HD21	1.98	0.45
1:F:190:ASN:O	1:F:191:LYS:C	2.54	0.45
1:F:287:GLU:O	1:F:291:ILE:HG13	2.16	0.45
1:C:81:TYR:CE2	1:C:110:LEU:HD21	2.52	0.45
1:E:95:LEU:HD13	1:E:96:GLY:N	2.32	0.45
1:F:144:ASN:ND2	1:F:160:PHE:CZ	2.85	0.45
1:A:215:ASN:ND2	1:A:319:ILE:CD1	2.72	0.45
1:C:92:LEU:HD12	1:C:107:ALA:CB	2.47	0.45
1:E:188:VAL:O	1:E:192:LEU:HG	2.16	0.45
1:E:298:LEU:CD1	1:E:303:THR:HG23	2.47	0.45
1:E:319:ILE:O	1:E:319:ILE:CG2	2.65	0.45
1:F:228:LYS:O	1:F:231:LYS:HE3	2.16	0.45
1:D:55:LEU:HD23	1:D:55:LEU:HA	1.85	0.44
1:D:179:HIS:C	1:D:181:ASP:N	2.68	0.44
1:F:173:THR:HG22	1:F:291:ILE:HG12	1.99	0.44
1:C:13:ARG:HB2	1:C:14:PRO:HD3	1.99	0.44
1:C:66:GLY:H	1:C:72:THR:HB	1.81	0.44
1:B:340:PRO:HG2	1:F:351:ASN:HB3	1.99	0.44
1:E:92:LEU:HD12	1:E:107:ALA:HB2	1.99	0.44
1:C:235:ILE:HG22	1:C:260:LEU:CG	2.40	0.44
1:F:195:GLU:HB2	1:F:198:GLN:HG3	1.99	0.44
1:B:180:ARG:O	1:B:181:ASP:C	2.56	0.44
1:B:252:GLU:O	1:B:253:PHE:C	2.55	0.44
1:C:209:ASN:ND2	1:C:319:ILE:HD11	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ASN:O	1:D:41:TYR:C	2.55	0.44
1:D:85:LEU:O	1:D:88:GLN:HG2	2.18	0.44
1:E:187:ASP:OD1	1:E:188:VAL:N	2.50	0.44
1:F:225:ASP:OD1	1:F:225:ASP:N	2.50	0.44
1:C:253:PHE:O	1:C:253:PHE:HD2	2.01	0.44
1:C:313:THR:O	1:C:313:THR:CG2	2.65	0.44
1:D:42:ASP:O	1:D:46:ASN:HB2	2.18	0.44
1:E:161:ASN:HD22	1:E:161:ASN:C	2.21	0.44
1:B:280:SER:OG	1:B:282:SER:HB3	2.17	0.44
1:C:260:LEU:HD23	1:C:260:LEU:HA	1.80	0.44
1:D:250:LYS:HA	1:D:252:GLU:OE1	2.18	0.44
1:A:307:GLU:OE1	1:A:307:GLU:N	2.46	0.44
1:D:265:PHE:CE1	1:D:269:ASN:ND2	2.86	0.44
1:E:40:ASN:O	1:E:43:TYR:HB3	2.17	0.44
1:D:80:THR:HG21	1:D:103:ALA:HB1	1.99	0.44
1:D:94:ILE:HD11	1:D:103:ALA:HB3	2.00	0.44
1:F:212:ASN:C	1:F:212:ASN:ND2	2.69	0.44
1:F:224:ASN:O	1:F:227:ALA:N	2.51	0.44
1:F:236:TYR:CE1	1:F:238:THR:HB	2.53	0.43
1:A:121:ASN:O	1:A:134:ARG:HD3	2.18	0.43
1:B:93:LEU:HD21	1:B:117:MET:HE2	2.00	0.43
1:B:137:VAL:HA	1:B:140:VAL:HG12	2.01	0.43
1:A:4:LEU:CD1	1:A:90:ASP:HB2	2.48	0.43
1:A:224:ASN:O	1:A:227:ALA:HB3	2.19	0.43
1:A:284:THR:O	1:A:288:GLU:HG3	2.18	0.43
1:C:8:THR:HG1	1:C:32:GLN:HE21	1.62	0.43
1:E:13:ARG:HD3	1:E:50:PHE:CZ	2.52	0.43
1:F:13:ARG:HD3	1:F:50:PHE:CE2	2.52	0.43
1:F:153:ARG:O	1:F:154:TYR:C	2.55	0.43
1:A:189:LEU:HD13	1:A:196:PRO:HD3	2.00	0.43
1:A:246:ILE:HD12	1:A:246:ILE:O	2.17	0.43
1:B:45:LEU:HD22	1:B:45:LEU:HA	1.89	0.43
1:D:209:ASN:ND2	1:D:299:ILE:O	2.51	0.43
1:D:352:VAL:O	1:D:356:VAL:HG23	2.18	0.43
1:A:45:LEU:HD22	1:A:45:LEU:O	2.19	0.43
1:B:121:ASN:O	1:B:134:ARG:HD3	2.18	0.43
1:C:33:ILE:HG22	1:C:33:ILE:O	2.18	0.43
1:D:161:ASN:HD22	1:D:161:ASN:C	2.22	0.43
1:D:202:VAL:HG22	1:D:279:LEU:HD13	2.01	0.43
1:D:247:GLU:HG2	1:D:251:PHE:CB	2.48	0.43
1:E:198:GLN:HA	1:E:198:GLN:NE2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:LYS:O	1:F:28:GLN:HG3	2.18	0.43
1:F:43:TYR:C	1:F:45:LEU:H	2.22	0.43
1:F:45:LEU:HD23	1:F:45:LEU:HA	1.88	0.43
1:F:251:PHE:O	1:F:252:GLU:C	2.57	0.43
1:B:144:ASN:ND2	1:B:160:PHE:CE2	2.87	0.43
1:B:230:TYR:HE1	1:B:332:ARG:HD3	1.83	0.43
1:B:319:ILE:HD13	1:B:319:ILE:HA	1.90	0.43
1:C:46:ASN:HD22	1:C:46:ASN:N	2.16	0.43
1:D:176:ILE:O	1:D:180:ARG:N	2.50	0.43
1:F:48:ILE:HG13	1:F:49:PHE:H	1.83	0.43
1:A:13:ARG:CB	1:A:14:PRO:HD3	2.48	0.43
1:A:48:ILE:O	1:A:53:LEU:HB2	2.18	0.43
1:A:73:MET:SD	1:B:109:ARG:HD2	2.59	0.43
1:B:334:MET:HG3	1:B:339:GLU:HG3	1.99	0.43
1:C:37:THR:HA	1:C:62:LEU:HB2	2.00	0.43
1:C:73:MET:HE1	1:D:109:ARG:HH11	1.84	0.43
1:C:183:ILE:HG22	1:C:184:ASN:ND2	2.34	0.43
1:E:207:GLU:C	1:E:208:GLU:CG	2.87	0.43
1:F:315:ILE:CD1	1:F:330:LEU:HB3	2.49	0.43
1:B:200:ILE:O	1:B:234:VAL:HA	2.18	0.43
1:D:286:SER:O	1:D:308:VAL:HG21	2.18	0.43
1:E:264:GLY:O	1:E:266:PHE:N	2.52	0.43
1:C:26:CYS:O	1:C:30:PHE:HB2	2.18	0.43
1:D:25:ALA:O	1:D:29:TYR:HD2	2.01	0.43
1:E:64:ALA:O	1:E:65:VAL:CB	2.65	0.43
1:E:290:SER:HB2	1:E:313:THR:HG21	2.01	0.43
1:C:92:LEU:HD12	1:C:107:ALA:HB2	2.01	0.43
1:D:322:ASN:C	1:D:322:ASN:ND2	2.68	0.43
1:A:72:THR:O	1:A:76:ILE:HG13	2.19	0.42
1:A:332:ARG:HA	1:A:332:ARG:HD2	1.37	0.42
1:B:253:PHE:O	1:B:254:ASP:CB	2.67	0.42
1:B:303:THR:HB	1:B:305:ARG:H	1.84	0.42
1:C:69:LEU:HA	1:C:72:THR:CG2	2.49	0.42
1:B:161:ASN:ND2	1:B:163:ALA:H	2.17	0.42
1:F:1:MET:O	1:F:2:GLU:OE1	2.37	0.42
1:F:334:MET:CG	1:F:339:GLU:HG3	2.45	0.42
1:A:339:GLU:HG2	1:C:354:THR:HG21	2.01	0.42
1:B:237:SER:HB3	1:B:260:LEU:HD12	2.00	0.42
1:D:81:TYR:CE2	1:D:110:LEU:HD21	2.54	0.42
1:D:247:GLU:HA	1:D:251:PHE:HB2	2.01	0.42
1:E:52:ASP:C	1:E:54:GLU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:PHE:CD1	1:E:335:GLN:NE2	2.87	0.42
1:E:319:ILE:O	1:E:319:ILE:HG22	2.20	0.42
1:F:13:ARG:HD3	1:F:50:PHE:CZ	2.55	0.42
1:A:164:ASN:HD22	1:A:164:ASN:N	2.18	0.42
1:C:45:LEU:H	1:C:45:LEU:HG	1.47	0.42
1:D:93:LEU:HD22	1:D:94:ILE:N	2.33	0.42
1:C:330:LEU:HD22	1:C:334:MET:HE1	2.01	0.42
1:D:40:ASN:O	1:D:42:ASP:N	2.52	0.42
1:D:219:LEU:O	1:D:222:ALA:HB3	2.20	0.42
1:F:220:MET:HE3	1:F:236:TYR:HE2	1.85	0.42
1:C:203:SER:HA	1:C:237:SER:O	2.19	0.42
1:E:80:THR:HA	1:E:83:VAL:HG12	2.02	0.42
1:D:358:LYS:HE3	1:F:334:MET:CE	2.45	0.42
1:F:48:ILE:HD12	1:F:49:PHE:CD2	2.54	0.42
1:F:49:PHE:O	1:F:52:ASP:O	2.38	0.42
1:F:94:ILE:HG22	1:F:116:HIS:HA	2.02	0.42
1:F:250:LYS:HE3	1:F:250:LYS:HB3	1.88	0.42
1:B:13:ARG:N	1:B:14:PRO:CD	2.82	0.42
1:B:329:GLU:OE2	1:B:332:ARG:NH1	2.52	0.42
1:C:62:LEU:O	1:C:63:GLU:C	2.57	0.42
1:A:319:ILE:O	1:A:320:THR:C	2.58	0.42
1:D:1:MET:SD	1:D:1:MET:N	2.89	0.42
1:D:230:TYR:HE1	1:D:332:ARG:HD3	1.83	0.42
1:E:115:PHE:CE2	1:E:360:ILE:HA	2.55	0.42
1:F:366:ILE:HG23	1:F:370:ASN:ND2	2.35	0.42
1:B:144:ASN:ND2	1:B:160:PHE:CZ	2.88	0.41
1:B:239:HIS:CB	1:B:240:PRO:HD2	2.49	0.41
1:B:369:ARG:O	1:B:373:ARG:HA	2.20	0.41
1:C:76:ILE:O	1:C:80:THR:OG1	2.29	0.41
1:C:329:GLU:O	1:C:333:GLU:HB2	2.20	0.41
1:D:319:ILE:HD13	1:D:319:ILE:HA	1.88	0.41
1:E:211:ASP:O	1:E:213:GLU:N	2.53	0.41
1:E:280:SER:CB	1:E:285:LEU:HG	2.50	0.41
1:F:62:LEU:O	1:F:64:ALA:N	2.52	0.41
1:A:49:PHE:CZ	1:A:58:PRO:HD3	2.55	0.41
1:B:4:LEU:C	1:B:4:LEU:HD23	2.41	0.41
1:C:93:LEU:HD21	1:C:117:MET:HE2	2.02	0.41
1:C:323:ASN:O	1:C:327:SER:OG	2.29	0.41
1:F:45:LEU:O	1:F:48:ILE:CG1	2.64	0.41
1:A:253:PHE:CD1	1:A:257:VAL:HG11	2.55	0.41
1:B:65:VAL:CA	1:B:72:THR:HB	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:LEU:C	1:C:47:GLN:N	2.73	0.41
1:C:225:ASP:O	1:C:229:LYS:HB2	2.20	0.41
1:B:225:ASP:N	1:B:225:ASP:OD1	2.53	0.41
1:C:131:GLU:HA	1:C:134:ARG:HD2	2.02	0.41
1:D:123:CYS:O	1:D:124:PHE:HB2	2.20	0.41
1:F:119:ALA:HB1	1:F:144:ASN:HB3	2.02	0.41
1:F:187:ASP:O	1:F:190:ASN:N	2.54	0.41
1:F:235:ILE:HG22	1:F:260:LEU:HG	2.02	0.41
1:D:369:ARG:NH1	1:F:301:THR:HB	2.35	0.41
1:A:78:ALA:O	1:A:81:TYR:HB3	2.20	0.41
1:E:19:LEU:HD11	1:E:95:LEU:HB2	2.03	0.41
1:A:26:CYS:O	1:A:30:PHE:HB2	2.20	0.41
1:B:334:MET:SD	1:F:354:THR:HG22	2.60	0.41
1:C:335:GLN:OE1	1:C:335:GLN:HA	2.21	0.41
1:D:64:ALA:O	1:D:65:VAL:CB	2.67	0.41
1:D:168:THR:O	1:D:352:VAL:HG22	2.20	0.41
1:F:50:PHE:CD2	1:F:50:PHE:N	2.87	0.41
1:A:347:TYR:N	1:A:347:TYR:CD1	2.89	0.41
1:B:7:MET:O	1:B:92:LEU:HA	2.21	0.41
1:B:260:LEU:HD23	1:B:260:LEU:HA	1.87	0.41
1:B:325:ILE:HG22	1:B:326:GLN:N	2.35	0.41
1:C:81:TYR:CE1	1:C:85:LEU:HD12	2.56	0.41
1:E:24:LYS:HE2	1:E:54:GLU:O	2.21	0.41
1:E:74:GLY:HA3	1:F:74:GLY:O	2.21	0.41
1:E:243:TRP:HA	1:E:246:ILE:HG13	2.02	0.41
1:B:342:ILE:HD12	1:F:351:ASN:OD1	2.21	0.41
1:F:330:LEU:O	1:F:331:ALA:C	2.59	0.41
1:A:143:VAL:O	1:A:143:VAL:HG12	2.21	0.40
1:B:64:ALA:O	1:B:65:VAL:HG12	2.21	0.40
1:B:92:LEU:HD12	1:B:107:ALA:HB2	2.03	0.40
1:C:144:ASN:ND2	1:C:160:PHE:CZ	2.89	0.40
1:D:13:ARG:N	1:D:14:PRO:CD	2.84	0.40
1:D:123:CYS:HB3	1:D:304:GLU:OE1	2.21	0.40
1:D:170:SER:OG	1:D:287:GLU:OE2	2.32	0.40
1:E:40:ASN:HB2	1:E:61:TYR:CD2	2.55	0.40
1:F:43:TYR:O	1:F:45:LEU:N	2.54	0.40
1:A:68:ASN:ND2	1:A:71:GLU:HB2	2.36	0.40
1:A:133:ASN:O	1:A:134:ARG:C	2.59	0.40
1:A:306:PRO:C	1:A:308:VAL:H	2.25	0.40
1:C:81:TYR:CZ	1:C:110:LEU:HD21	2.56	0.40
1:E:66:GLY:O	1:E:67:SER:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:PHE:CE1	1:F:269:ASN:ND2	2.87	0.40
1:A:170:SER:HA	1:A:171:PRO:HD3	1.96	0.40
1:B:188:VAL:HG13	1:B:189:LEU:N	2.36	0.40
1:B:251:PHE:CD1	1:B:251:PHE:O	2.74	0.40
1:D:207:GLU:O	1:D:208:GLU:HG3	2.20	0.40
1:F:64:ALA:O	1:F:65:VAL:CB	2.69	0.40
1:F:183:ILE:HG22	1:F:184:ASN:ND2	2.37	0.40
1:B:330:LEU:HD22	1:B:334:MET:CE	2.51	0.40
1:C:118:GLU:HG3	1:C:147:TYR:CE2	2.56	0.40
1:C:207:GLU:O	1:C:208:GLU:CB	2.69	0.40
1:C:224:ASN:OD1	1:C:253:PHE:HA	2.20	0.40
1:D:66:GLY:O	1:D:67:SER:C	2.60	0.40
1:D:253:PHE:CE1	1:D:257:VAL:HG11	2.57	0.40
1:D:363:TYR:HA	1:D:366:ILE:HB	2.02	0.40
1:E:40:ASN:OD1	1:E:43:TYR:HB3	2.21	0.40
1:E:284:THR:O	1:E:285:LEU:C	2.60	0.40
1:F:76:ILE:O	1:F:80:THR:HB	2.22	0.40
1:F:116:HIS:CE1	1:F:119:ALA:HA	2.56	0.40
1:A:306:PRO:C	1:A:308:VAL:N	2.75	0.40
1:F:176:ILE:CG2	1:F:292:LEU:HD21	2.52	0.40
1:F:202:VAL:HA	1:F:279:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/374 (98%)	301 (82%)	55 (15%)	12 (3%)	4	25
1	B	372/374 (100%)	305 (82%)	50 (13%)	17 (5%)	2	18
1	C	372/374 (100%)	311 (84%)	45 (12%)	16 (4%)	2	20
1	D	372/374 (100%)	312 (84%)	46 (12%)	14 (4%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	372/374 (100%)	306 (82%)	52 (14%)	14 (4%)	3	22
1	F	372/374 (100%)	299 (80%)	55 (15%)	18 (5%)	2	17
All	All	2228/2244 (99%)	1834 (82%)	303 (14%)	91 (4%)	3	21

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	134	ARG
1	A	140	VAL
1	A	252	GLU
1	A	254	ASP
1	B	65	VAL
1	B	215	ASN
1	B	253	PHE
1	B	254	ASP
1	B	293	LYS
1	C	43	TYR
1	C	162	LYS
1	C	188	VAL
1	C	248	GLU
1	C	252	GLU
1	D	41	TYR
1	D	42	ASP
1	D	65	VAL
1	D	67	SER
1	D	69	LEU
1	D	373	ARG
1	E	65	VAL
1	E	69	LEU
1	E	212	ASN
1	E	265	PHE
1	E	285	LEU
1	E	293	LYS
1	F	2	GLU
1	F	47	GLN
1	F	53	LEU
1	F	191	LYS
1	F	254	ASP
1	F	314	VAL
1	A	136	ILE

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Mol	Chain	Res	Type
1	A	247	GLU
1	A	248	GLU
1	B	64	ALA
1	B	69	LEU
1	B	107	ALA
1	B	188	VAL
1	C	11	GLY
1	C	41	TYR
1	C	53	LEU
1	C	65	VAL
1	C	264	GLY
1	D	180	ARG
1	D	208	GLU
1	D	253	PHE
1	E	67	SER
1	E	188	VAL
1	F	11	GLY
1	F	43	TYR
1	F	44	THR
1	F	65	VAL
1	F	252	GLU
1	A	251	PHE
1	B	249	SER
1	B	264	GLY
1	C	2	GLU
1	C	46	ASN
1	C	253	PHE
1	D	11	GLY
1	D	249	SER
1	E	231	LYS
1	F	20	SER
1	F	94	ILE
1	A	11	GLY
1	A	37	THR
1	A	307	GLU
1	B	11	GLY
1	B	214	LYS
1	D	2	GLU
1	D	212	ASN
1	D	254	ASP
1	E	284	THR
1	E	373	ARG

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Mol	Chain	Res	Type
1	F	63	GLU
1	B	330	LEU
1	C	182	LYS
1	E	11	GLY
1	E	254	ASP
1	F	86	ARG
1	F	224	ASN
1	B	325	ILE
1	C	254	ASP
1	F	48	ILE
1	B	136	ILE
1	B	299	ILE
1	E	235	ILE
1	F	74	GLY
1	C	235	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/341 (99%)	288 (85%)	51 (15%)	3	14
1	B	341/341 (100%)	290 (85%)	51 (15%)	3	14
1	C	341/341 (100%)	280 (82%)	61 (18%)	2	9
1	D	341/341 (100%)	286 (84%)	55 (16%)	2	11
1	E	341/341 (100%)	284 (83%)	57 (17%)	2	10
1	F	341/341 (100%)	281 (82%)	60 (18%)	2	9
All	All	2044/2046 (100%)	1709 (84%)	335 (16%)	2	11

All (335) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	43	TYR
1	A	45	LEU

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Mol	Chain	Res	Type
1	A	49	PHE
1	A	51	ASP
1	A	52	ASP
1	A	53	LEU
1	A	55	LEU
1	A	59	ASP
1	A	65	VAL
1	A	68	ASN
1	A	69	LEU
1	A	80	THR
1	A	92	LEU
1	A	93	LEU
1	A	95	LEU
1	A	101	CYS
1	A	109	ARG
1	A	138	ASP
1	A	140	VAL
1	A	162	LYS
1	A	208	GLU
1	A	214	LYS
1	A	215	ASN
1	A	219	LEU
1	A	220	MET
1	A	237	SER
1	A	241	ARG
1	A	242	SER
1	A	246	ILE
1	A	247	GLU
1	A	248	GLU
1	A	252	GLU
1	A	253	PHE
1	A	260	LEU
1	A	261	LYS
1	A	285	LEU
1	A	298	LEU
1	A	299	ILE
1	A	303	THR
1	A	311	LYS
1	A	313	THR
1	A	314	VAL
1	A	323	ASN
1	A	325	ILE

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Mol	Chain	Res	Type
1	A	332	ARG
1	A	333	GLU
1	A	334	MET
1	A	338	ASN
1	A	343	ASP
1	A	354	THR
1	B	1	MET
1	B	6	LEU
1	B	15	GLU
1	B	39	GLN
1	B	45	LEU
1	B	51	ASP
1	B	55	LEU
1	B	59	ASP
1	B	65	VAL
1	B	69	LEU
1	B	72	THR
1	B	80	THR
1	B	85	LEU
1	B	92	LEU
1	B	93	LEU
1	B	95	LEU
1	B	109	ARG
1	B	161	ASN
1	B	180	ARG
1	B	192	LEU
1	B	198	GLN
1	B	203	SER
1	B	205	HIS
1	B	209	ASN
1	B	213	GLU
1	B	218	SER
1	B	220	MET
1	B	225	ASP
1	B	232	MET
1	B	237	SER
1	B	242	SER
1	B	244	LYS
1	B	245	LYS
1	B	250	LYS
1	B	254	ASP
1	B	256	LEU

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Mol	Chain	Res	Type
1	B	263	PHE
1	B	286	SER
1	B	290	SER
1	B	298	LEU
1	B	303	THR
1	B	308	VAL
1	B	314	VAL
1	B	324	LEU
1	B	325	ILE
1	B	330	LEU
1	B	332	ARG
1	B	335	GLN
1	B	345	ILE
1	B	364	LYS
1	B	365	ASP
1	C	1	MET
1	C	6	LEU
1	C	16	ILE
1	C	39	GLN
1	C	41	TYR
1	C	44	THR
1	C	45	LEU
1	C	46	ASN
1	C	47	GLN
1	C	48	ILE
1	C	56	ARG
1	C	73	MET
1	C	85	LEU
1	C	92	LEU
1	C	93	LEU
1	C	95	LEU
1	C	97	ASP
1	C	101	CYS
1	C	109	ARG
1	C	138	ASP
1	C	142	ASP
1	C	161	ASN
1	C	173	THR
1	C	177	GLU
1	C	180	ARG
1	C	187	ASP
1	C	191	LYS

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Mol	Chain	Res	Type
1	C	195	GLU
1	C	201	LEU
1	C	207	GLU
1	C	210	ILE
1	C	220	MET
1	C	221	ASN
1	C	232	MET
1	C	236	TYR
1	C	242	SER
1	C	249	SER
1	C	251	PHE
1	C	253	PHE
1	C	254	ASP
1	C	260	LEU
1	C	261	LYS
1	C	266	PHE
1	C	282	SER
1	C	284	THR
1	C	285	LEU
1	C	298	LEU
1	C	299	ILE
1	C	303	THR
1	C	308	VAL
1	C	313	THR
1	C	314	VAL
1	C	319	ILE
1	C	325	ILE
1	C	330	LEU
1	C	332	ARG
1	C	334	MET
1	C	336	ASN
1	C	364	LYS
1	C	365	ASP
1	C	369	ARG
1	D	1	MET
1	D	21	SER
1	D	40	ASN
1	D	42	ASP
1	D	46	ASN
1	D	48	ILE
1	D	52	ASP
1	D	56	ARG

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Mol	Chain	Res	Type
1	D	59	ASP
1	D	69	LEU
1	D	72	THR
1	D	77	ILE
1	D	92	LEU
1	D	93	LEU
1	D	94	ILE
1	D	97	ASP
1	D	101	CYS
1	D	109	ARG
1	D	127	ASN
1	D	161	ASN
1	D	180	ARG
1	D	181	ASP
1	D	184	ASN
1	D	205	HIS
1	D	210	ILE
1	D	212	ASN
1	D	218	SER
1	D	220	MET
1	D	237	SER
1	D	246	ILE
1	D	250	LYS
1	D	251	PHE
1	D	252	GLU
1	D	253	PHE
1	D	254	ASP
1	D	258	LYS
1	D	261	LYS
1	D	273	LYS
1	D	280	SER
1	D	284	THR
1	D	285	LEU
1	D	286	SER
1	D	298	LEU
1	D	303	THR
1	D	308	VAL
1	D	313	THR
1	D	314	VAL
1	D	322	ASN
1	D	330	LEU
1	D	332	ARG

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Mol	Chain	Res	Type
1	D	334	MET
1	D	335	GLN
1	D	345	ILE
1	D	364	LYS
1	D	367	ILE
1	E	1	MET
1	E	2	GLU
1	E	6	LEU
1	E	46	ASN
1	E	47	GLN
1	E	49	PHE
1	E	55	LEU
1	E	56	ARG
1	E	59	ASP
1	E	65	VAL
1	E	69	LEU
1	E	92	LEU
1	E	93	LEU
1	E	94	ILE
1	E	100	SER
1	E	109	ARG
1	E	142	ASP
1	E	145	LEU
1	E	161	ASN
1	E	180	ARG
1	E	181	ASP
1	E	184	ASN
1	E	188	VAL
1	E	191	LYS
1	E	201	LEU
1	E	203	SER
1	E	207	GLU
1	E	208	GLU
1	E	212	ASN
1	E	217	LYS
1	E	218	SER
1	E	220	MET
1	E	232	MET
1	E	236	TYR
1	E	238	THR
1	E	239	HIS
1	E	242	SER

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Mol	Chain	Res	Type
1	E	247	GLU
1	E	250	LYS
1	E	253	PHE
1	E	260	LEU
1	E	261	LYS
1	E	263	PHE
1	E	280	SER
1	E	285	LEU
1	E	298	LEU
1	E	303	THR
1	E	304	GLU
1	E	308	VAL
1	E	314	VAL
1	E	324	LEU
1	E	330	LEU
1	E	334	MET
1	E	335	GLN
1	E	345	ILE
1	E	364	LYS
1	E	367	ILE
1	F	1	MET
1	F	6	LEU
1	F	37	THR
1	F	39	GLN
1	F	41	TYR
1	F	42	ASP
1	F	47	GLN
1	F	55	LEU
1	F	57	GLN
1	F	69	LEU
1	F	85	LEU
1	F	92	LEU
1	F	93	LEU
1	F	94	ILE
1	F	95	LEU
1	F	97	ASP
1	F	100	SER
1	F	109	ARG
1	F	142	ASP
1	F	145	LEU
1	F	157	ASP
1	F	161	ASN

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Mol	Chain	Res	Type
1	F	177	GLU
1	F	187	ASP
1	F	191	LYS
1	F	198	GLN
1	F	212	ASN
1	F	216	PHE
1	F	220	MET
1	F	224	ASN
1	F	225	ASP
1	F	232	MET
1	F	236	TYR
1	F	239	HIS
1	F	241	ARG
1	F	242	SER
1	F	244	LYS
1	F	245	LYS
1	F	246	ILE
1	F	249	SER
1	F	250	LYS
1	F	253	PHE
1	F	257	VAL
1	F	260	LEU
1	F	266	PHE
1	F	292	LEU
1	F	298	LEU
1	F	299	ILE
1	F	303	THR
1	F	308	VAL
1	F	314	VAL
1	F	319	ILE
1	F	322	ASN
1	F	324	LEU
1	F	330	LEU
1	F	334	MET
1	F	335	GLN
1	F	354	THR
1	F	365	ASP
1	F	369	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	31	ASN
1	A	68	ASN
1	A	161	ASN
1	A	164	ASN
1	A	198	GLN
1	A	209	ASN
1	A	215	ASN
1	A	259	GLN
1	A	338	ASN
1	A	361	GLN
1	B	46	ASN
1	B	47	GLN
1	B	161	ASN
1	B	164	ASN
1	B	184	ASN
1	B	326	GLN
1	B	336	ASN
1	B	361	GLN
1	C	32	GLN
1	C	46	ASN
1	C	47	GLN
1	C	57	GLN
1	C	75	ASN
1	C	161	ASN
1	C	184	ASN
1	C	198	GLN
1	C	205	HIS
1	C	209	ASN
1	C	322	ASN
1	C	326	GLN
1	D	28	GLN
1	D	32	GLN
1	D	40	ASN
1	D	75	ASN
1	D	161	ASN
1	D	164	ASN
1	D	184	ASN
1	D	212	ASN
1	D	224	ASN
1	D	322	ASN
1	D	326	GLN
1	D	336	ASN

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Mol	Chain	Res	Type
1	E	28	GLN
1	E	32	GLN
1	E	39	GLN
1	E	47	GLN
1	E	161	ASN
1	E	164	ASN
1	E	184	ASN
1	E	198	GLN
1	E	205	HIS
1	E	212	ASN
1	E	326	GLN
1	E	335	GLN
1	E	336	ASN
1	F	28	GLN
1	F	39	GLN
1	F	75	ASN
1	F	116	HIS
1	F	161	ASN
1	F	164	ASN
1	F	184	ASN
1	F	198	GLN
1	F	212	ASN
1	F	224	ASN
1	F	322	ASN
1	F	323	ASN
1	F	326	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	372/374 (99%)	-0.58	0	100	100	32, 60, 105, 136	0
1	B	374/374 (100%)	-0.54	0	100	100	34, 65, 122, 161	0
1	C	374/374 (100%)	-0.47	5 (1%)	77	65	35, 69, 115, 144	0
1	D	374/374 (100%)	-0.42	3 (0%)	86	78	35, 66, 124, 189	0
1	E	374/374 (100%)	-0.43	3 (0%)	86	78	42, 69, 129, 179	0
1	F	374/374 (100%)	-0.44	3 (0%)	86	78	41, 74, 125, 185	0
All	All	2242/2244 (99%)	-0.48	14 (0%)	89	83	32, 67, 121, 189	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	41	TYR	3.7
1	D	251	PHE	3.5
1	F	41	TYR	3.2
1	C	1	MET	3.0
1	C	41	TYR	3.0
1	D	44	THR	2.8
1	D	41	TYR	2.8
1	E	252	GLU	2.7
1	E	45	LEU	2.7
1	C	67	SER	2.3
1	F	252	GLU	2.3
1	F	40	ASN	2.2
1	C	338	ASN	2.2
1	C	43	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.